

OPTION A: ANALYTICAL CHEM

A3 — INFRARED (IR)

SPECTROSCOPY

IB Chemistry
TAD02



A3 – Infrared (IR) Spectroscopy

- A.3.1 Describe the operating principles of a double-beam IR spectrometer. (2) *A schematic diagram of a simple double-beam spectrometer is sufficient.*
- A.3.2 Describe how information from an IR spectrum can be used to identify bonds. (2)
- A.3.3 Explain what occurs at a molecular level during the absorption of IR radiation by molecules. (3) *H₂O, –CH₂–, SO₂ and CO₂ are suitable examples. Stress the change in bond polarity as the vibrations (stretching and bending) occur.*
- A.3.4 Analyze IR spectra of organic compounds. (3) *Students will be assessed using examples containing up to three functional groups. The Chemistry data booklet contains a table of IR absorptions for some bonds in organic molecules. Students should realize that IR absorption data can be used to identify the bonds present, but not always the functional groups present.*



Why IR?

- Infrared (IR) radiation is just below the frequency of red in the electromagnetic spectrum
- IR radiation is not energetic enough to cause the promotion of electrons into an electronic excited state, the molecules will increase in vibrational energy instead

Frequency dependent on

- Strength of bond
- Masses of atoms

Two main uses

- Identify functional groups
- Identify substances

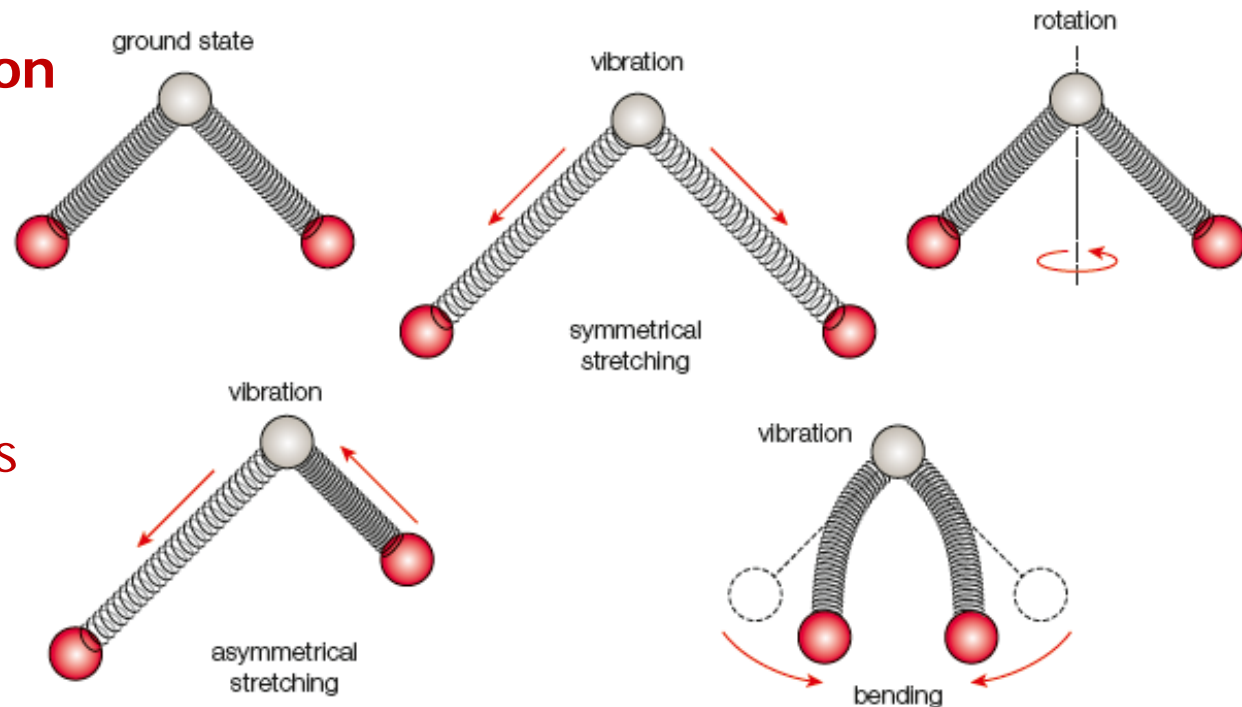
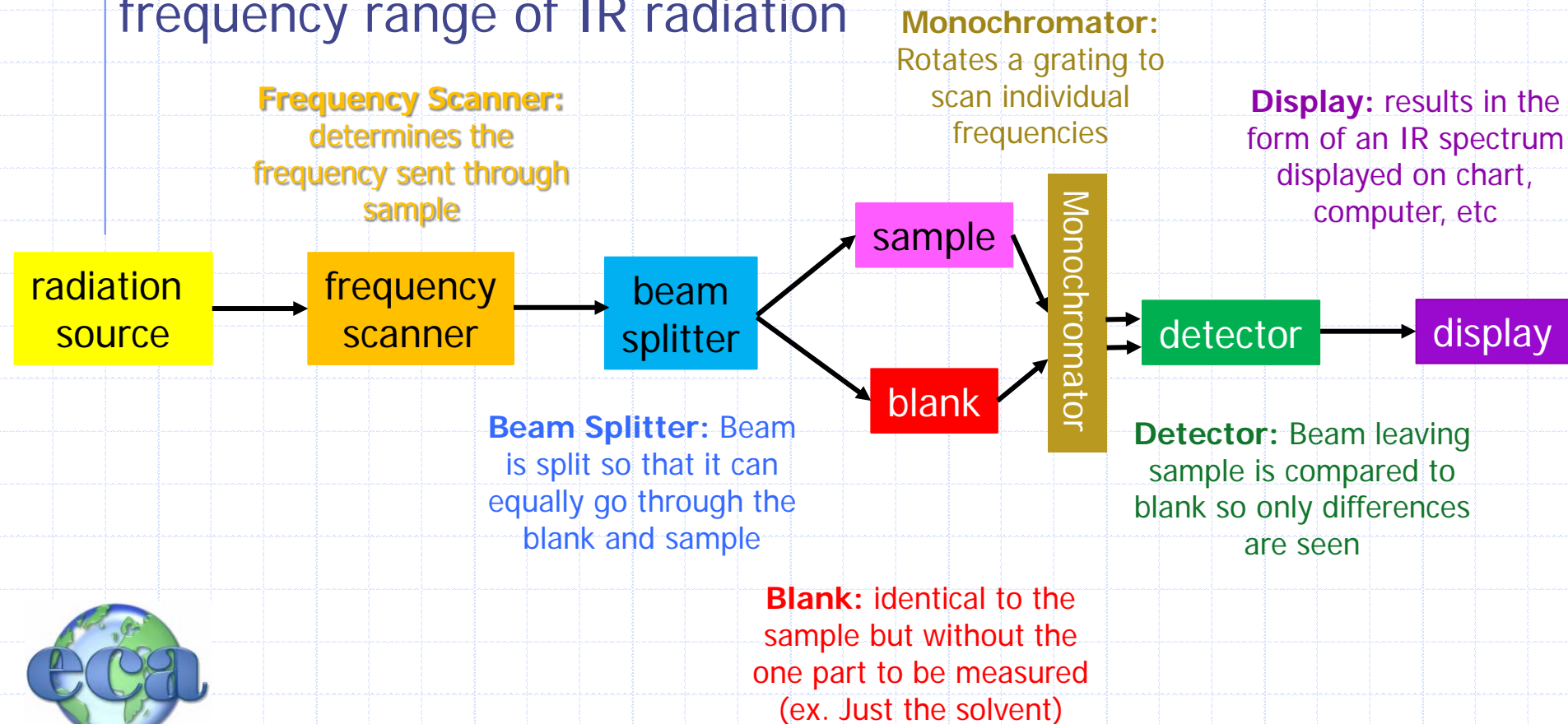


Figure 21.19 Vibrational and rotational motion in a triatomic molecule



A.3.1 Describe the operating principles of a double-beam IR spectrometer. (2)

- An IR spectrometer measures the extent to which infrared radiation is absorbed by a sample over a particular frequency range of IR radiation



Description of IR Parts

- **Radiation Source:**

- - A heated filament produces IR radiation

- **Beam Splitter:**

- Beam is split into two parallel beams
 - One through the sample to be studied
 - One through the reference sample
 - Allows for correction from H_2O and CO_2 in the atmosphere

- Mirrors direct the IR beams so they follow a parallel path

- **Monochromator** grating

- Diffraction grating splits up IR into separate frequencies
- The grating is rotated to direct IR of each frequency to the detector which records their intensities

- **Detector:**

- Converts radiation into an electrical signal

Compares the intensity of the beam from sample and blank

Determines the absorption at particular frequencies



IR Diagram

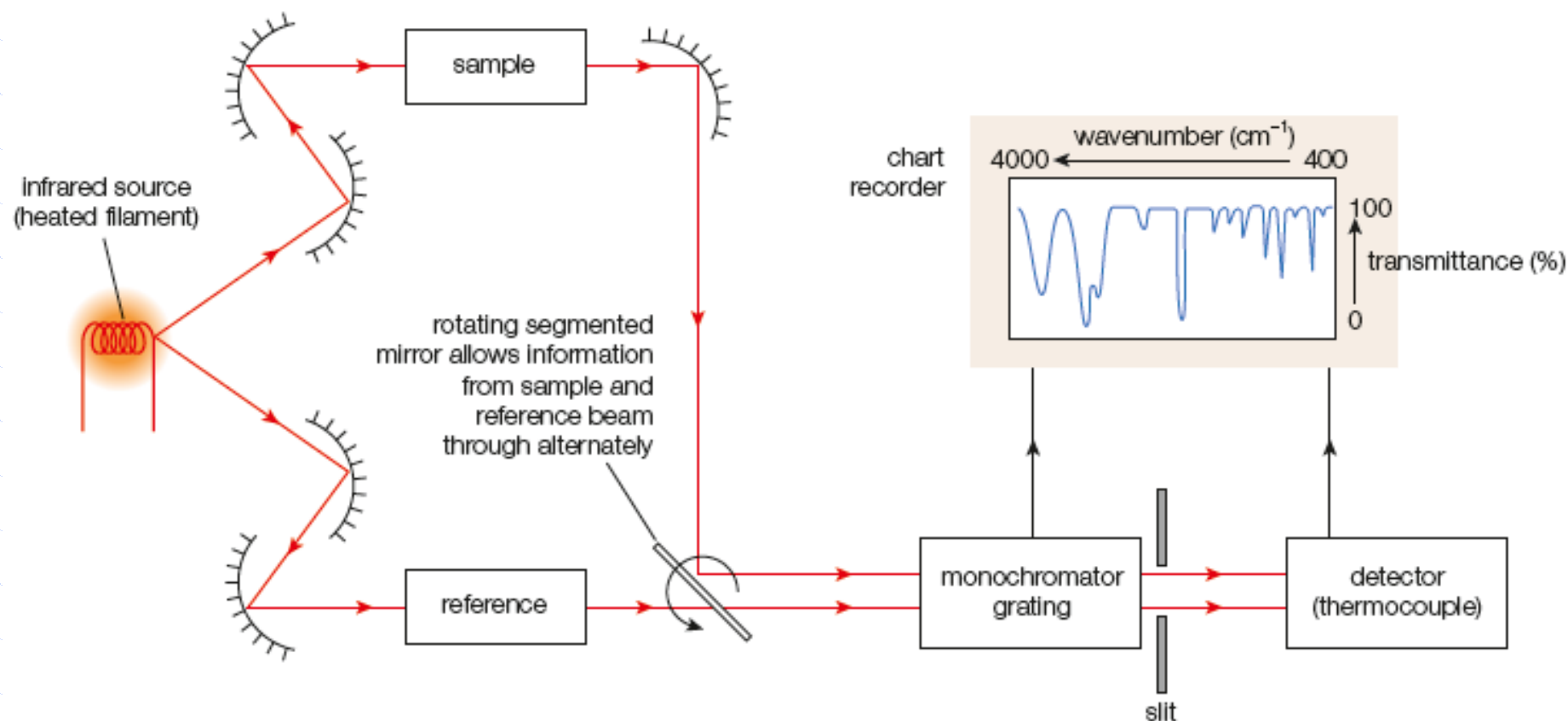


Figure 21.21 The essential optics and components of a double-beam infrared spectrometer

Bond Identification via IR

A.3.2 Describe how information from an IR spectrum can be used to identify bonds. (2)

- A table listing the common bonds/functional groups identified by IR can be found in your IB Data Booklet

Bond	Organic Molecules	Wavenumber (cm ⁻¹)
C-I	Iodoalkanes	490-620
C-Br	Bromoalkanes	500-600
C-Cl	Chloroalkanes	600-800
C-F	Fluroalkanes	1000-1400
C-O	Alcohols, esters, ethers	1050-1410
C=C	Alkenes	1610-1680
C=O	Aldehydes, ketones, acids, esters	1700-1750
C(triple)C	Alkynes	2100-2260
O-H	'Hydrogen bonded' in acids	2500-3300
C-H	Alkanes, Alkenes, Arenes	2850-3100
O-H	'Hydrogen bonded" in alcohols, phenols	3200-3600
N-H	Primary amines	3300-3500

Approach to IR Spectra

- Examine the spectrum from left to right starting at 4000 cm^{-1}
- Note which are the strongest absorptions and attempt to match them from the data booklet
- Note absence of peaks in important areas
- Do not attempt to match all the peaks, the fingerprint region ($<1500\text{ cm}^{-1}$) may cause some frustrations

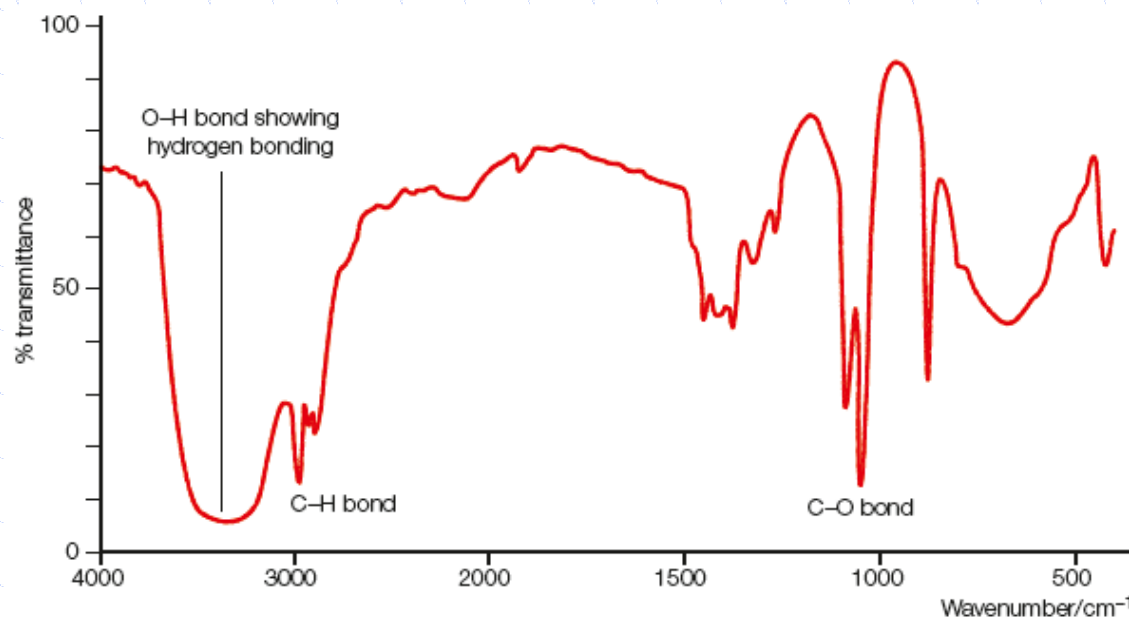


Figure 21.24 The infrared spectrum of ethanol



Alcohol vs Ketone

Figure 21.30

IR spectrum of methanol

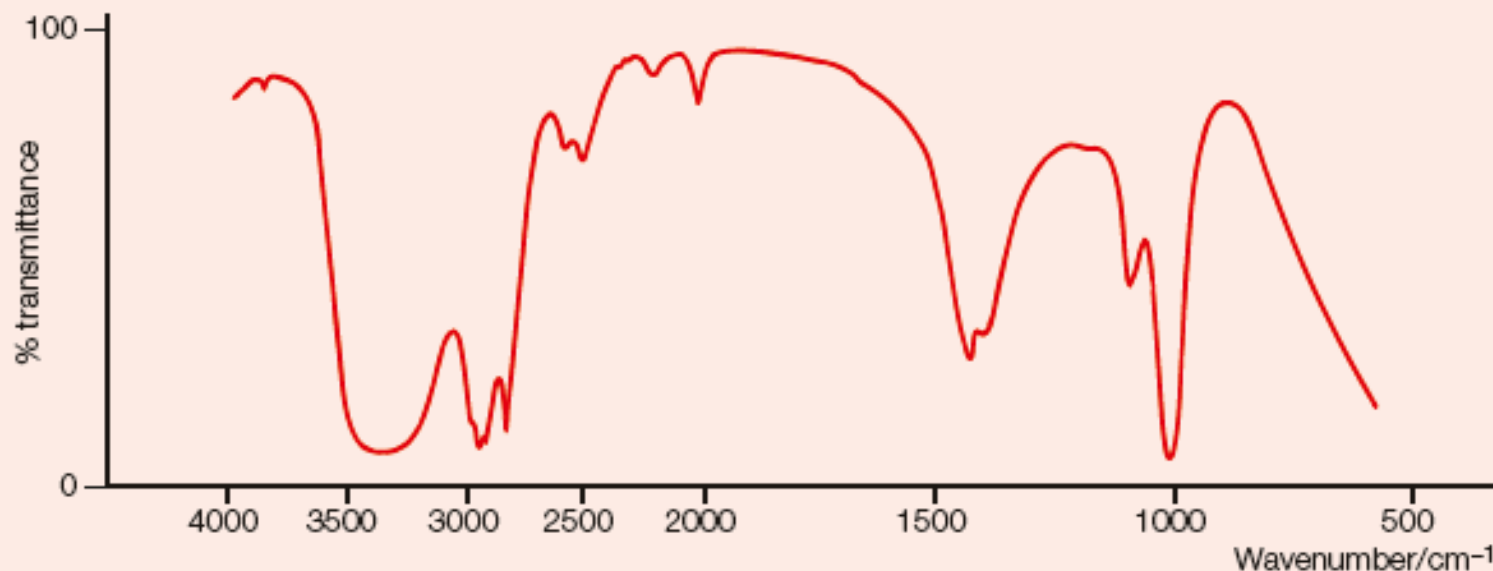
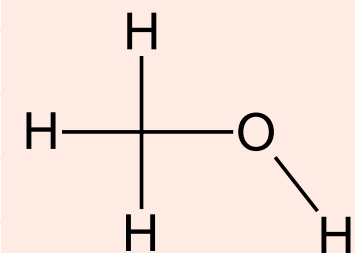
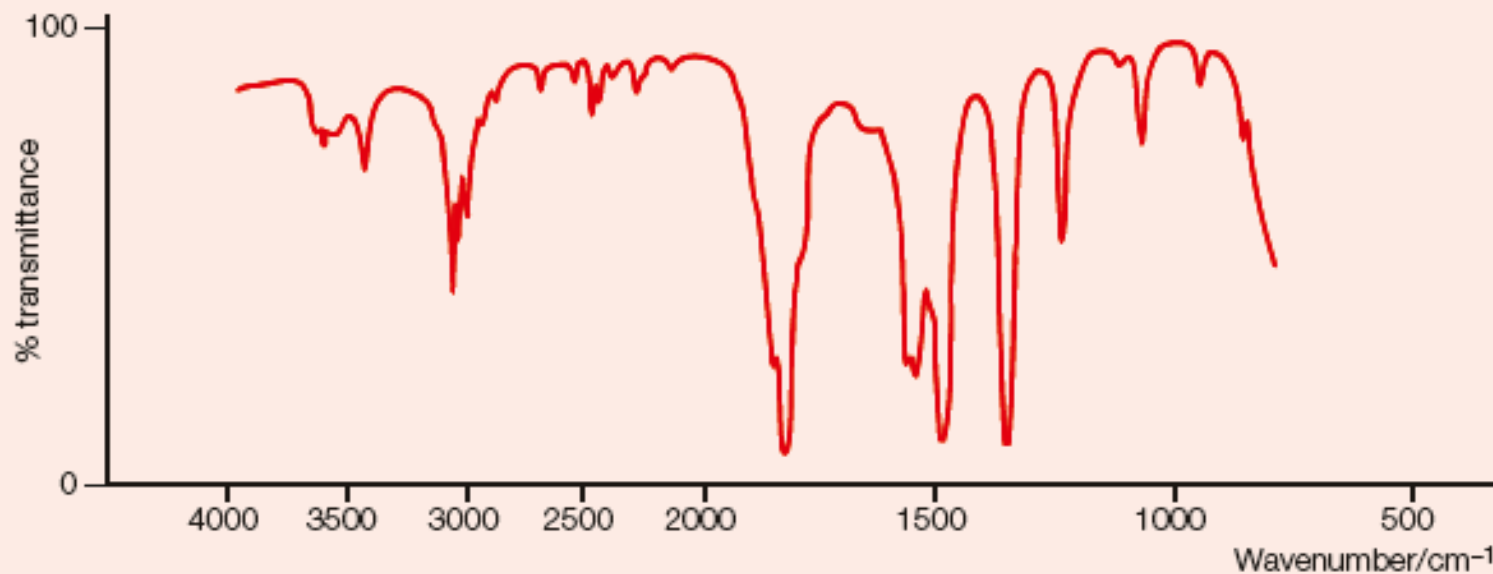
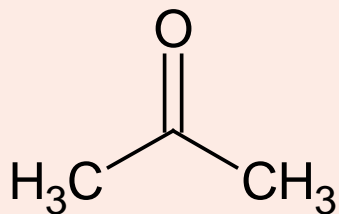


Figure 21.31

IR spectrum of propanone



CO₂ and H₂O

Figure 21.34
IR spectrum of carbon
dioxide

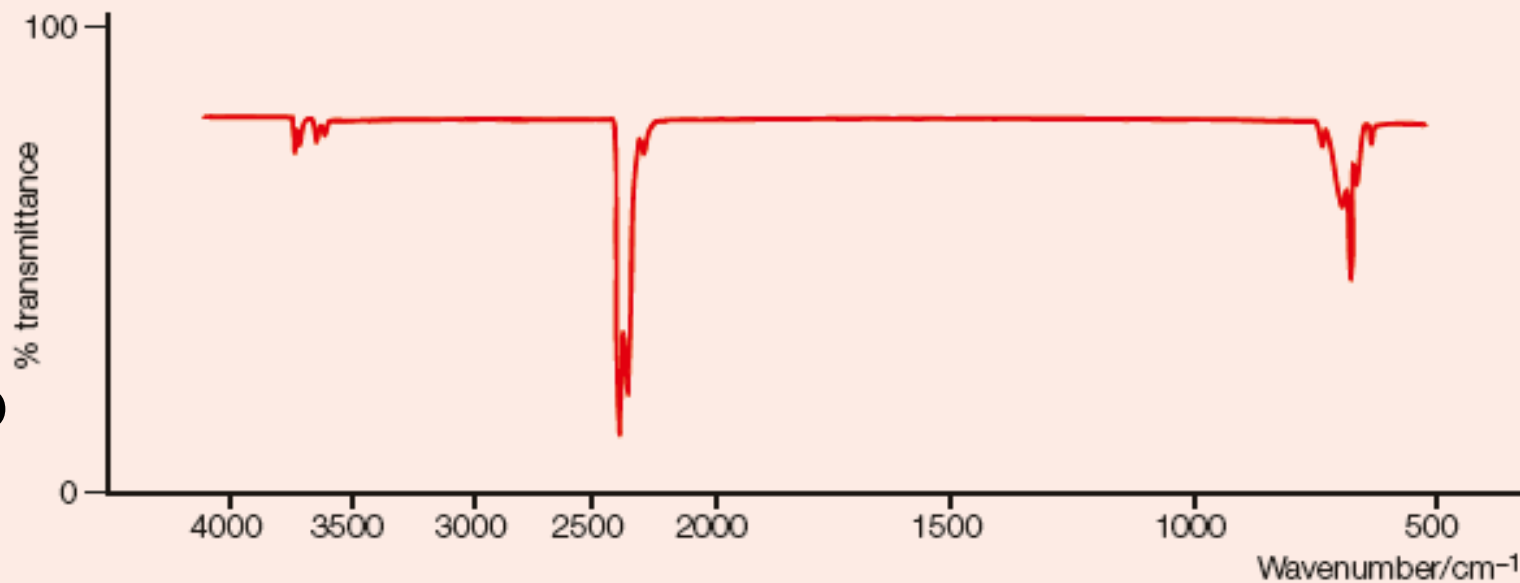
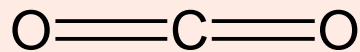
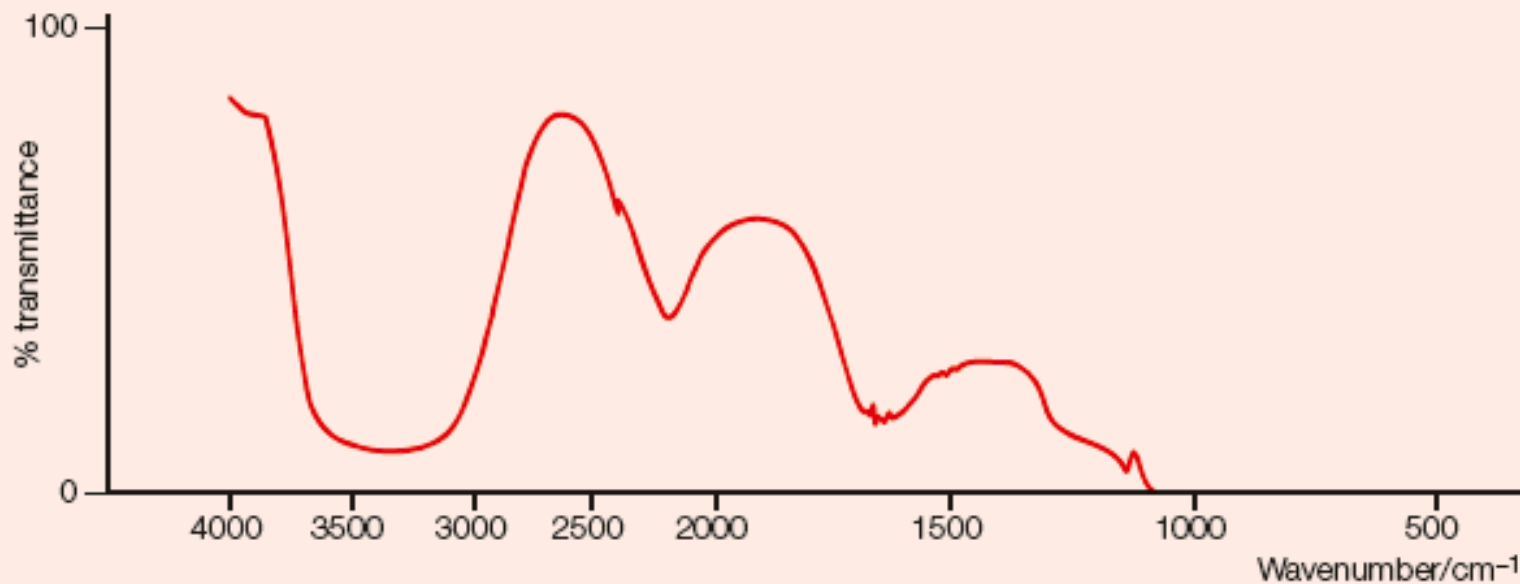
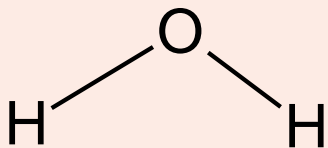


Figure 21.35
IR spectrum of water



Aliphatic vs Arene

Figure 21.26
IR spectrum of hexane

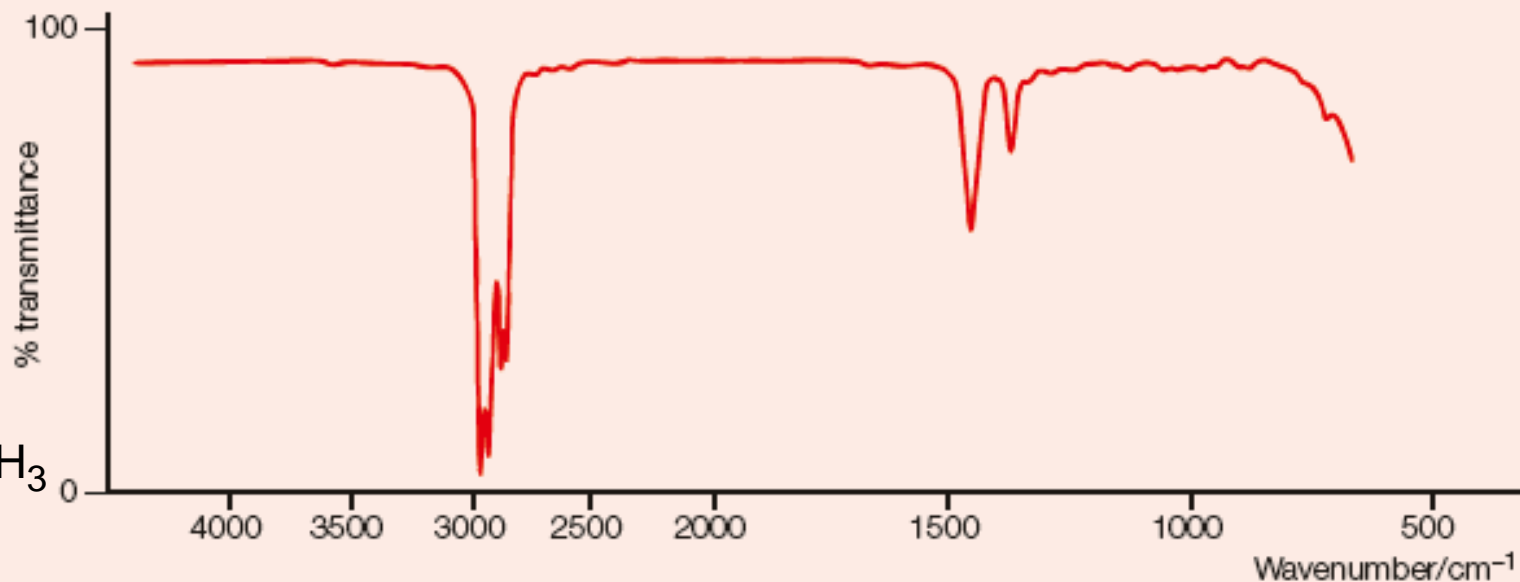
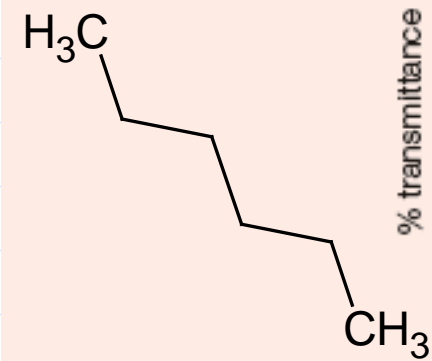
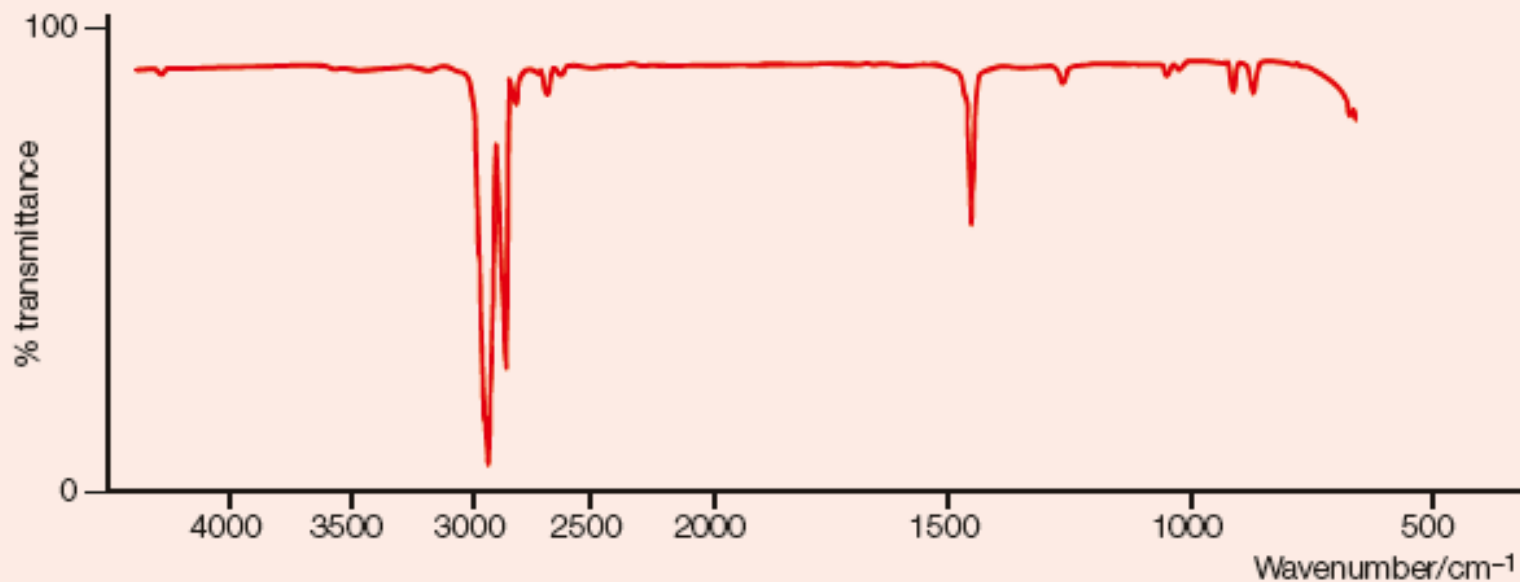
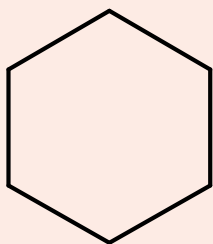


Figure 21.27
IR spectrum of cyclohexane



IR Absorption Example

- Vitamin C (ascorbic acid) contains C, H, and O atoms. What structural information can be deduced about its structure from the labeled absorption bands below?

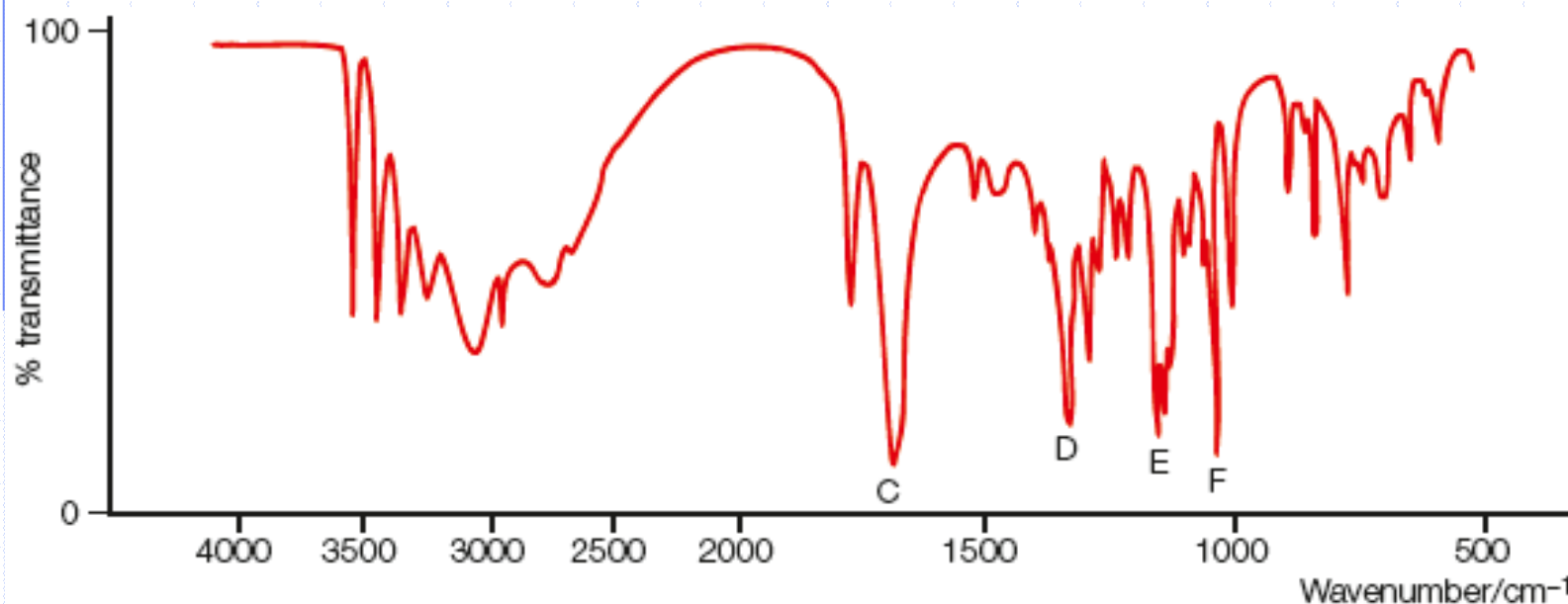


Figure 21.37 IR spectrum of vitamin C

Band C (Carbonyl C=O or C=C)

Bands D,E,F (C-O)

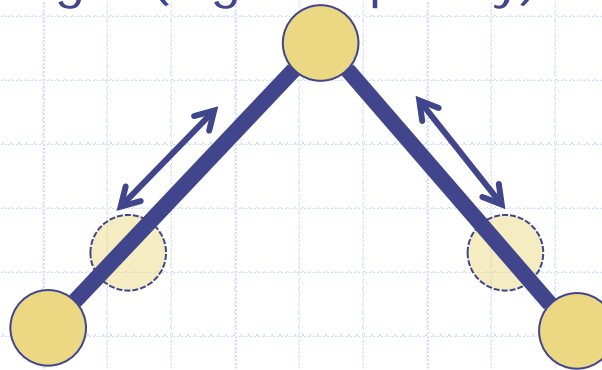
Bands E or F (C-C possible)



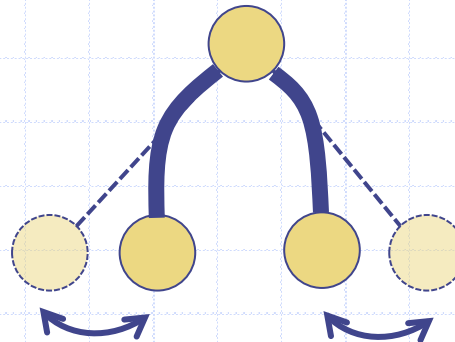
IR Molecular Action

A.3.3 Explain what occurs at a molecular level during the absorption of IR radiation by molecules. (3)

- Two types of IR excitation can occur:
 - **Bond stretching**
 - Requires more energy than bending and will therefore absorb in the shorter wavelength (high frequency) region



- **Bond bending**



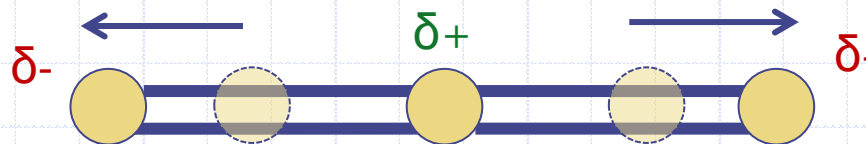
What can IR see?

- **IR Active Molecules:** In order to be IR active, the molecule must undergo a change in dipole moment (electrical charge altered)
 - NOT ALL vibrations will be seen in the IR region.
 - Diatomic elements (O_2 , H_2 , etc)
 - Those that are active
 - Diatomic compounds: with TWO DIFFERENT elements (halides, etc)
 - Triatomic compounds: various modes of vibration possible but must still undergo a change in dipole moment

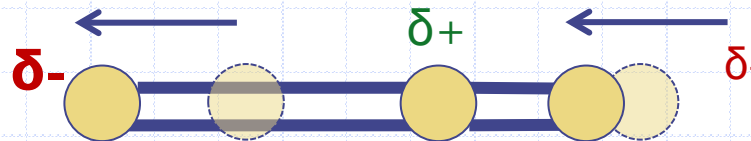


CO₂ Stretching

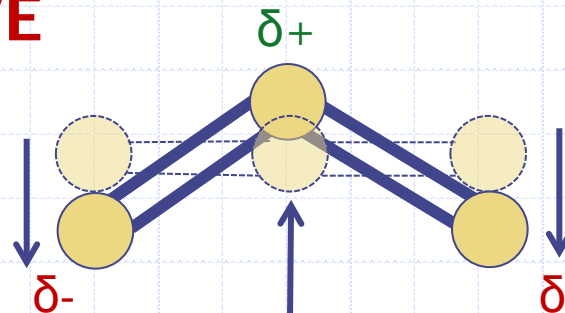
- Symmetrical Stretch: NOT ACTIVE



- Asymmetrical Stretch: **ACTIVE**

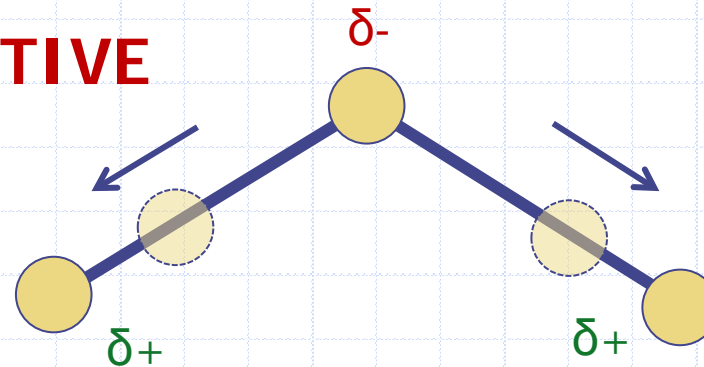


- Bending: **ACTIVE**

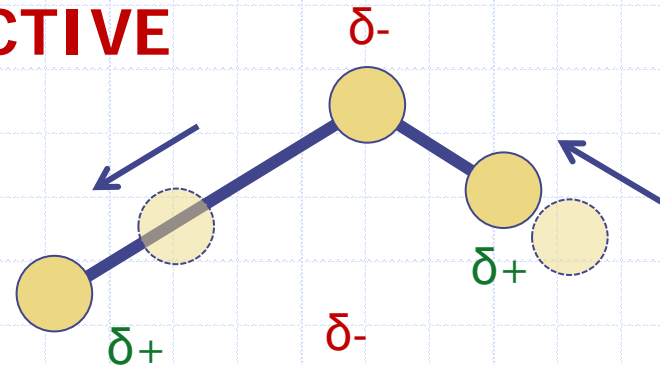


H₂O Stretching / Bending

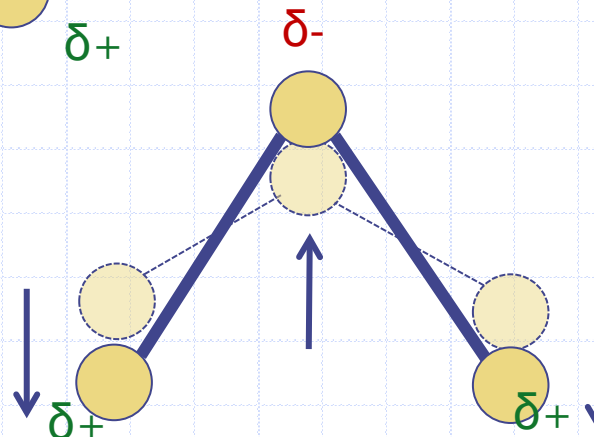
- Symmetrical Stretch: **ACTIVE**



- Asymmetrical Stretch: **ACTIVE**

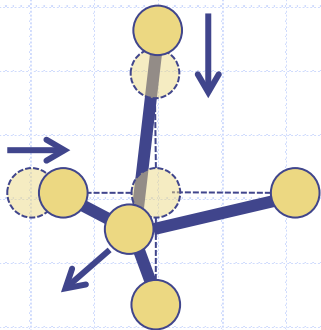


- Bending: **ACTIVE**

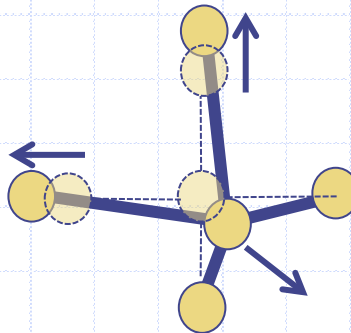


CH₄ Stretching / Bending

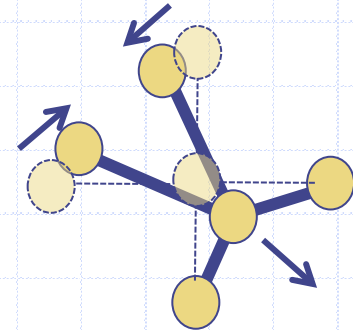
- With 4 terminal atoms, many possibilities exist



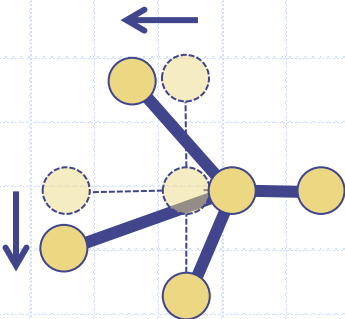
Asymmetric Stretching:
ACTIVE



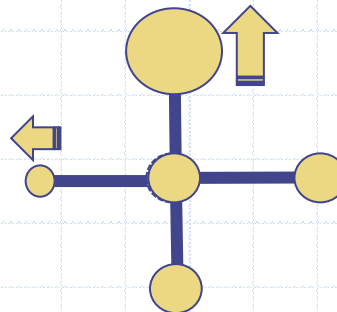
Symmetric Stretching:
ACTIVE



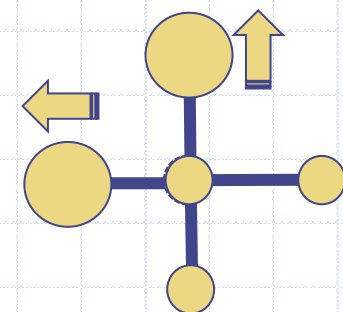
Bending/Scissoring:
NOT ACTIVE



Rocking or
in-plane bending:
NOT ACTIVE



Twisting or
out-of-plane bending:
NOT ACTIVE



Wagging or
out-of-plane bending:
NOT ACTIVE



Analyzing IR Data

A.3.4 Analyze IR spectra of organic compounds. (3)

- When analyzing IR Data
 - Use the IB data booklet
 - Scan left to right (begin with 4000 – 1300 nm^{-1} range)



Things to watch out for...

Look for a carbonyl in the region 1760-1690. If there is such a band:

Indicates:

Is an O-H band also present?

a carboxylic acid group

Is a C-O band also present?

an ester

Is an aldehydic C-H band also present?

an aldehyde

Is an N-H band also present?

an amide

Are none of the above present?

a ketone

Look for a broad O-H band in the region 3500-3200 cm^{-1} . If there is such a band:

Indicates:

Is an O-H band present?

an alcohol or phenol

Look for a single or double sharp N-H band in the region 3400-3250 cm^{-1} .
If there is such a band:

Indicates:

Are there two bands?

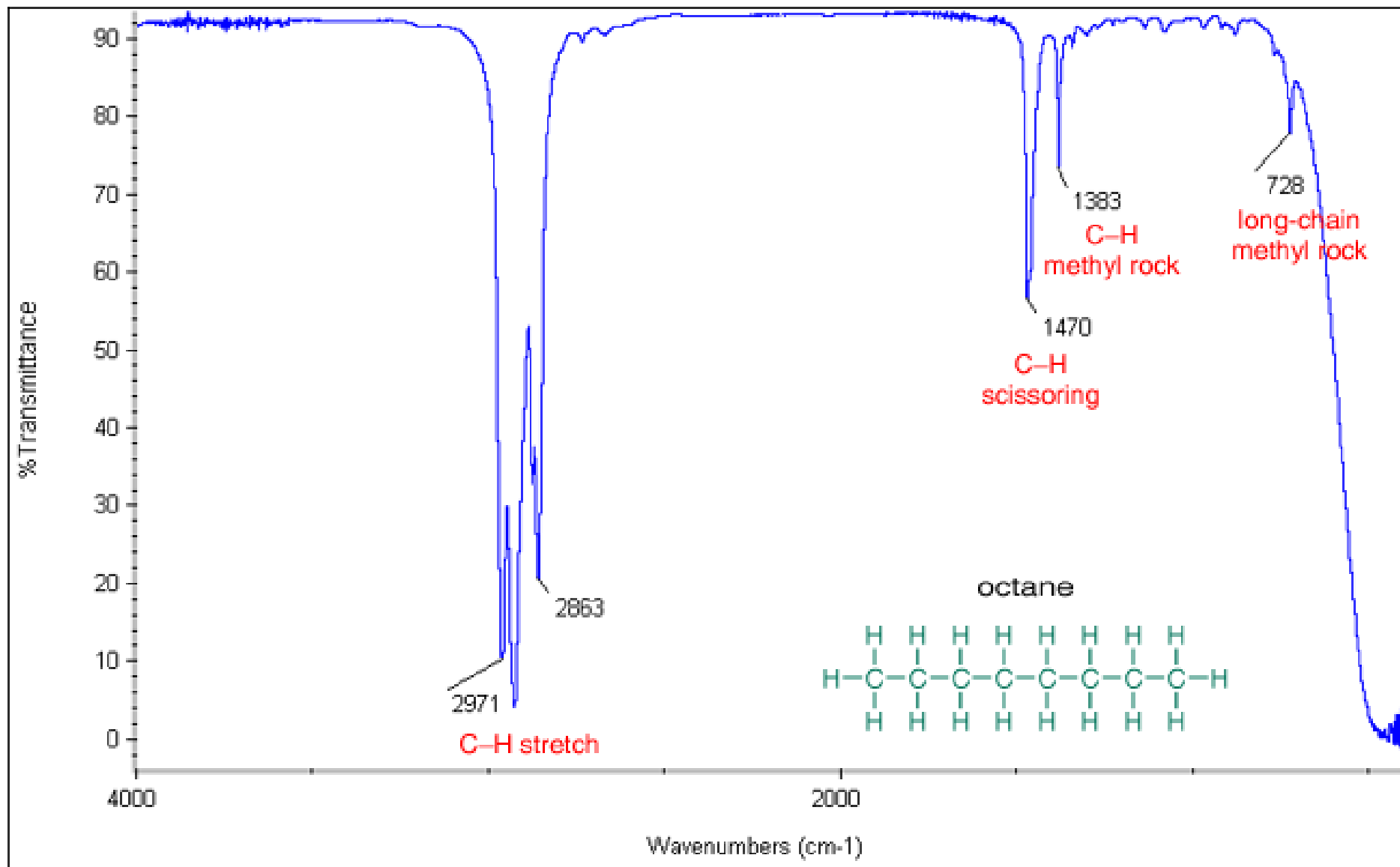
a primary amine

Is there only one band?

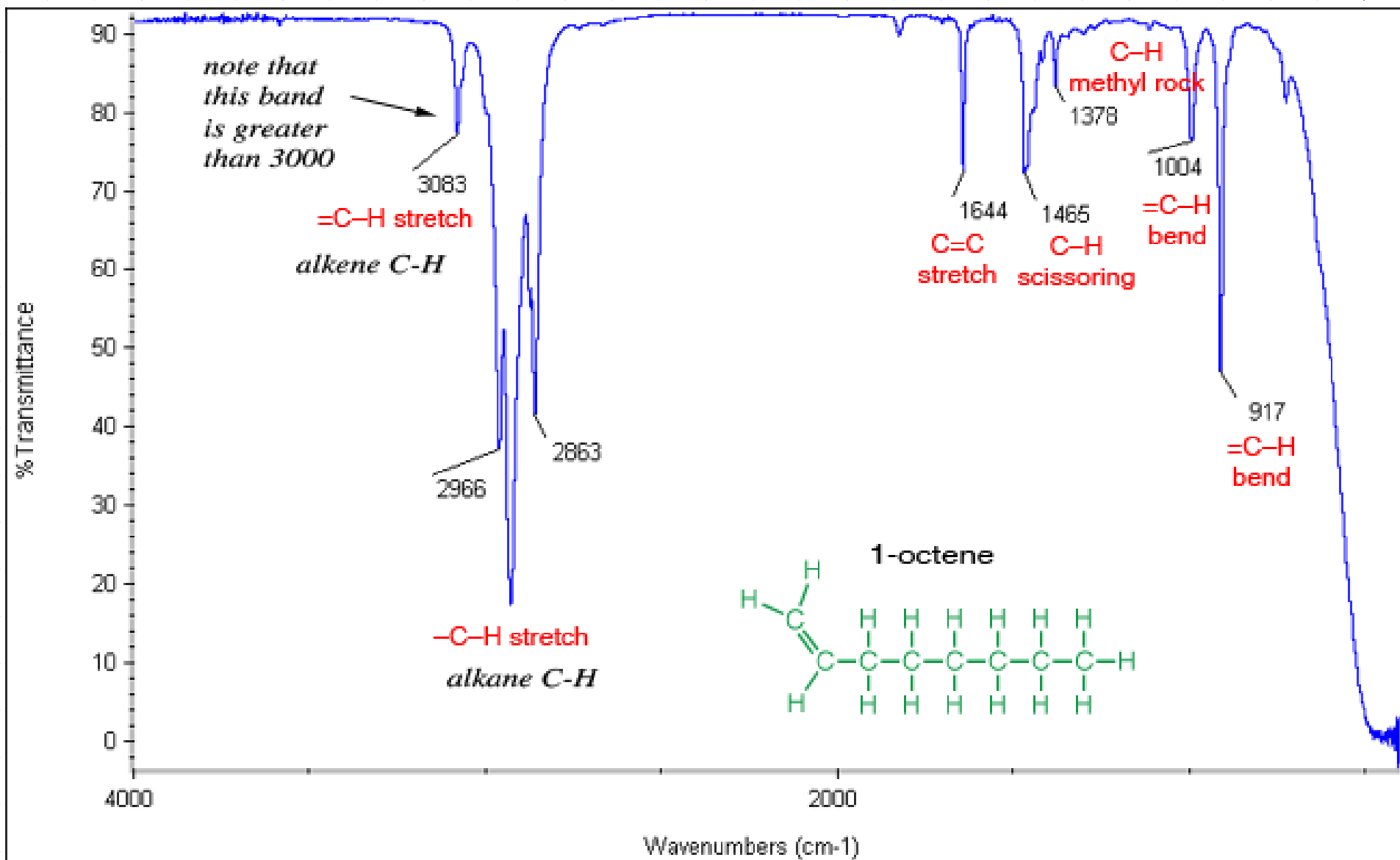
a secondary amine



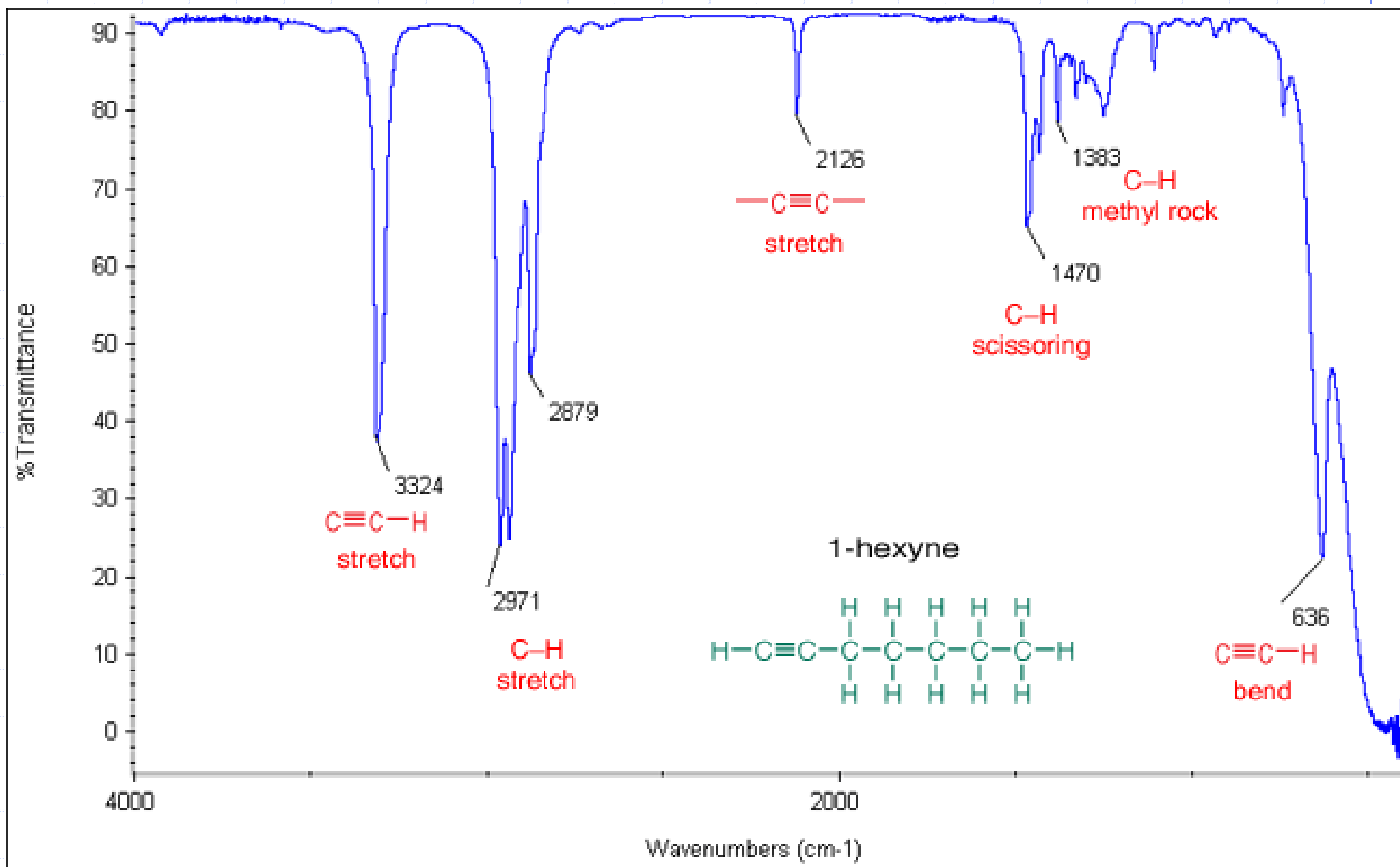
Alkane IR Data



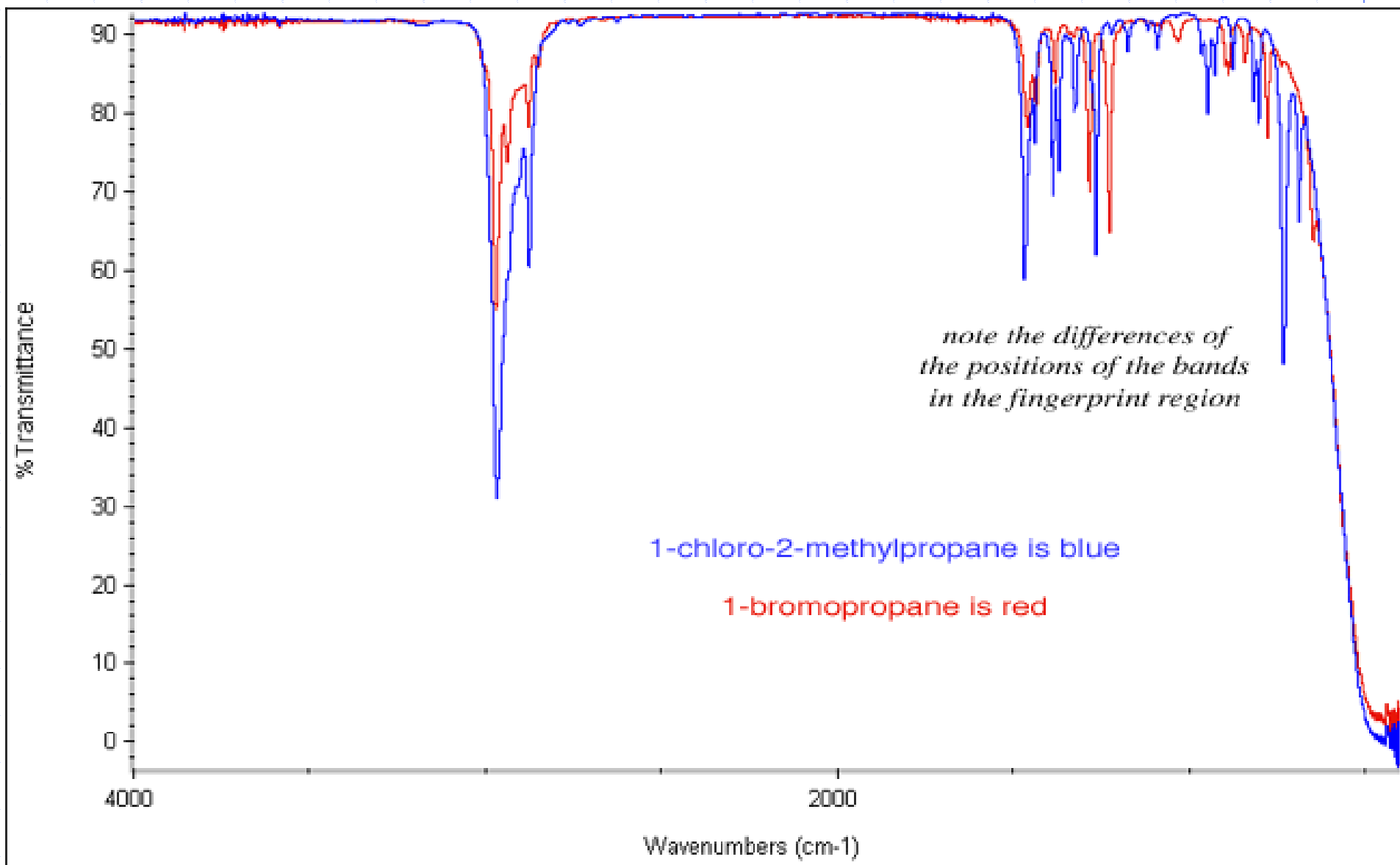
Alkene IR Data



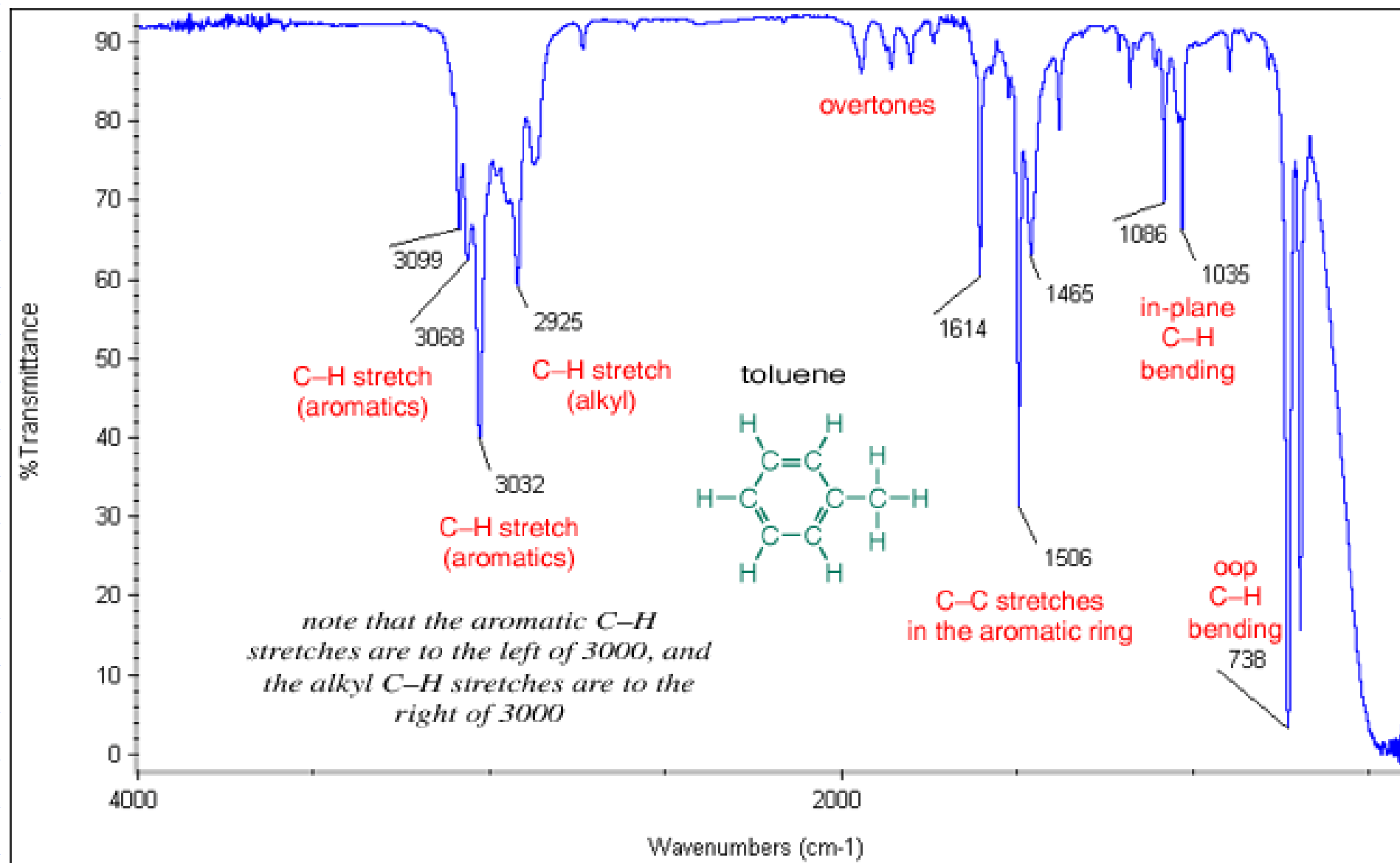
Alkyne IR Data



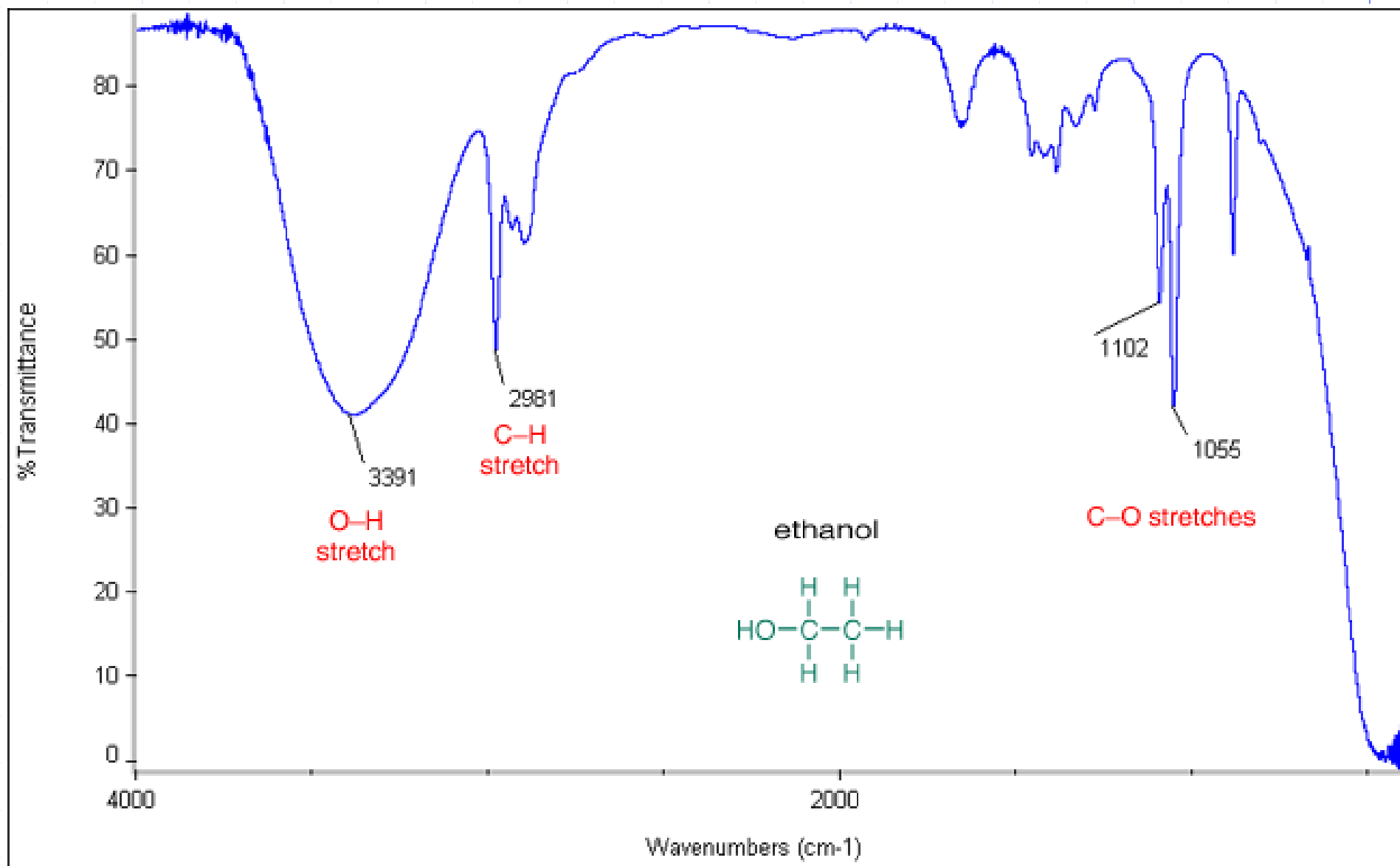
Halide IR Data



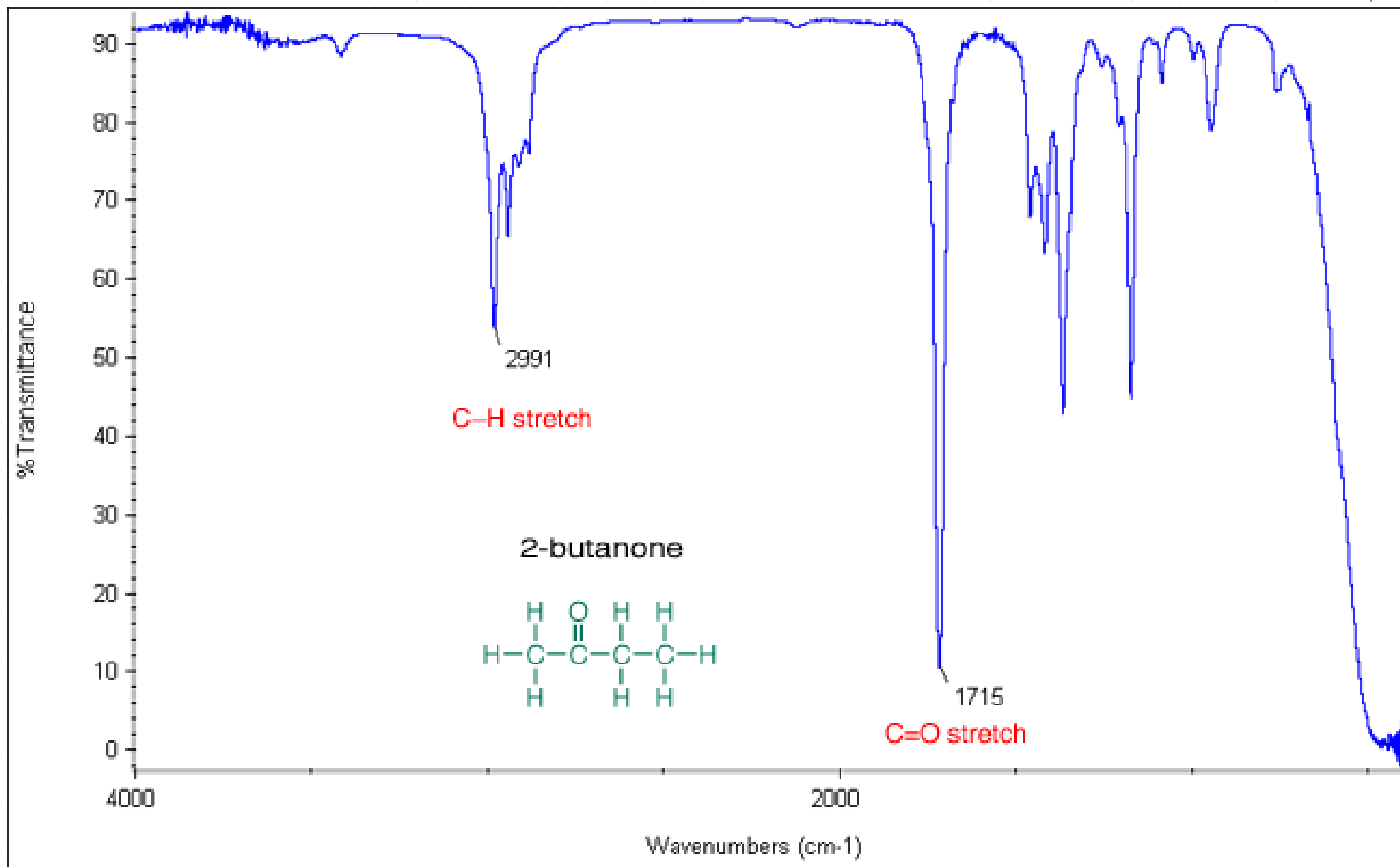
Aromatic IR Data



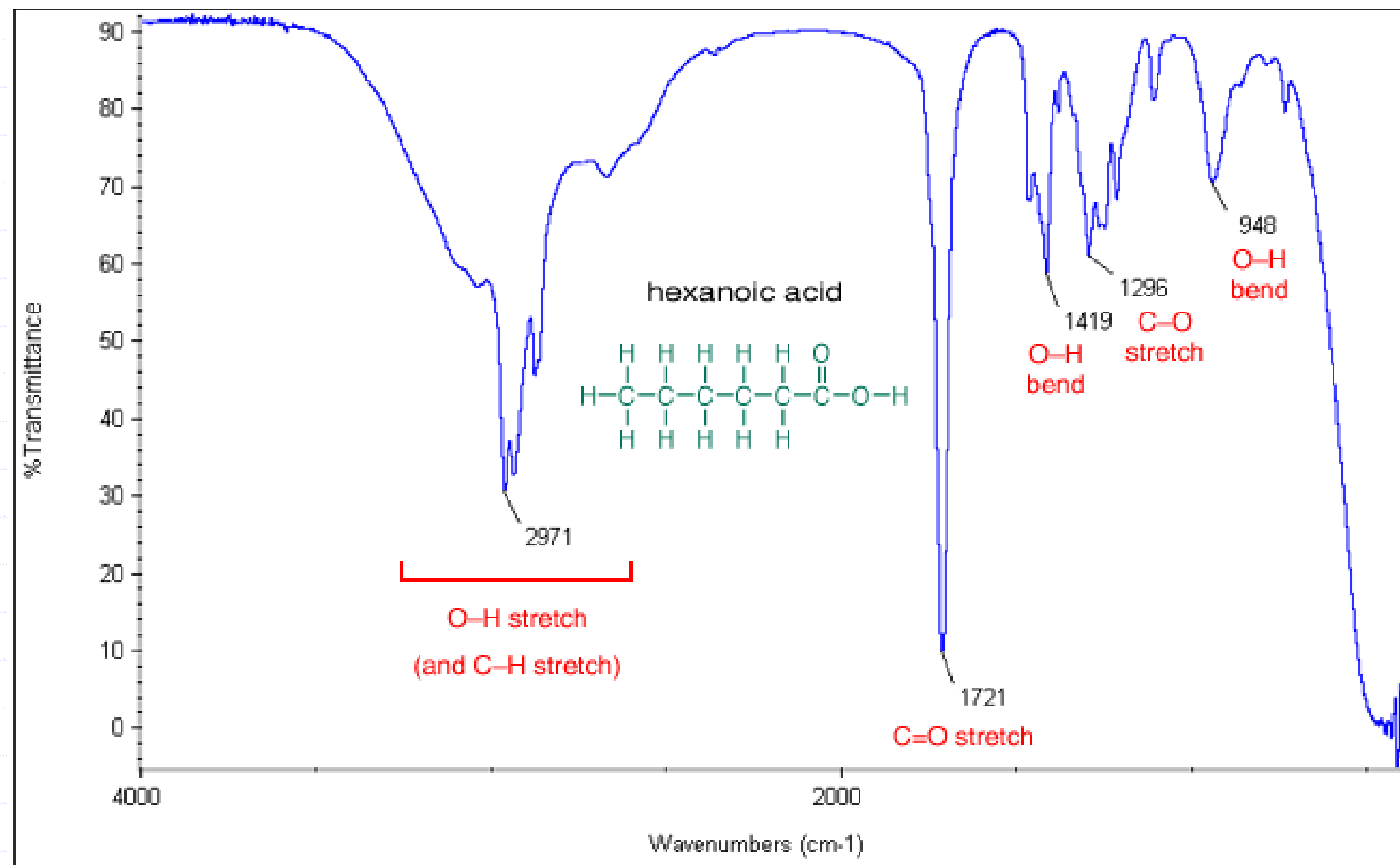
Alcohol IR Data



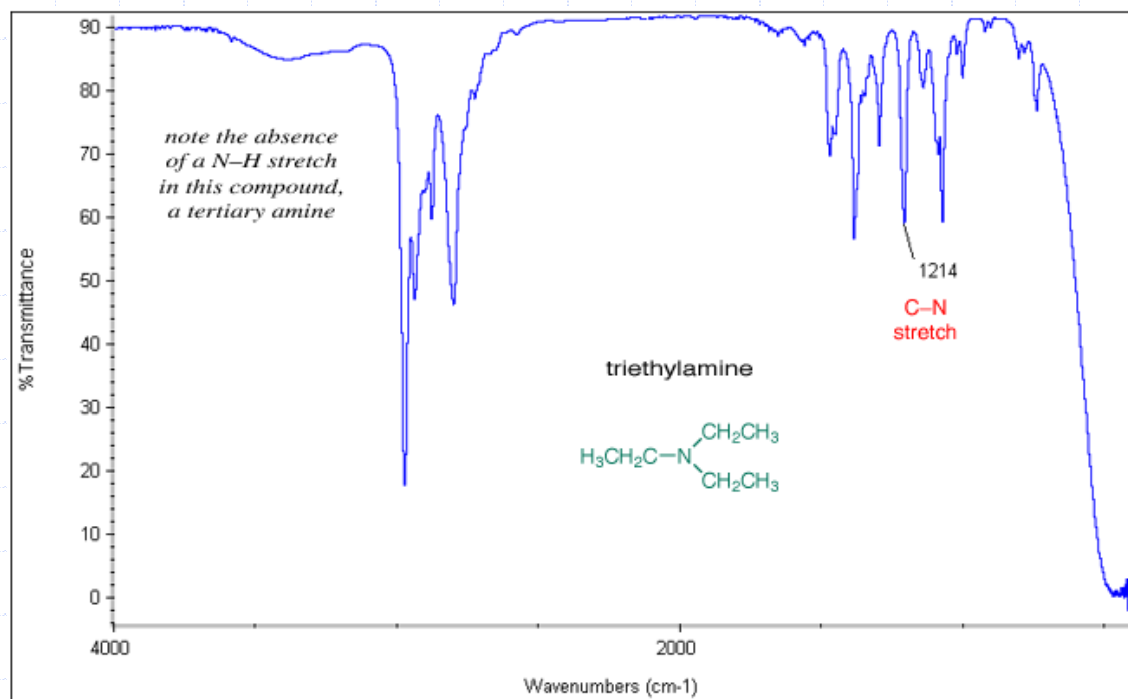
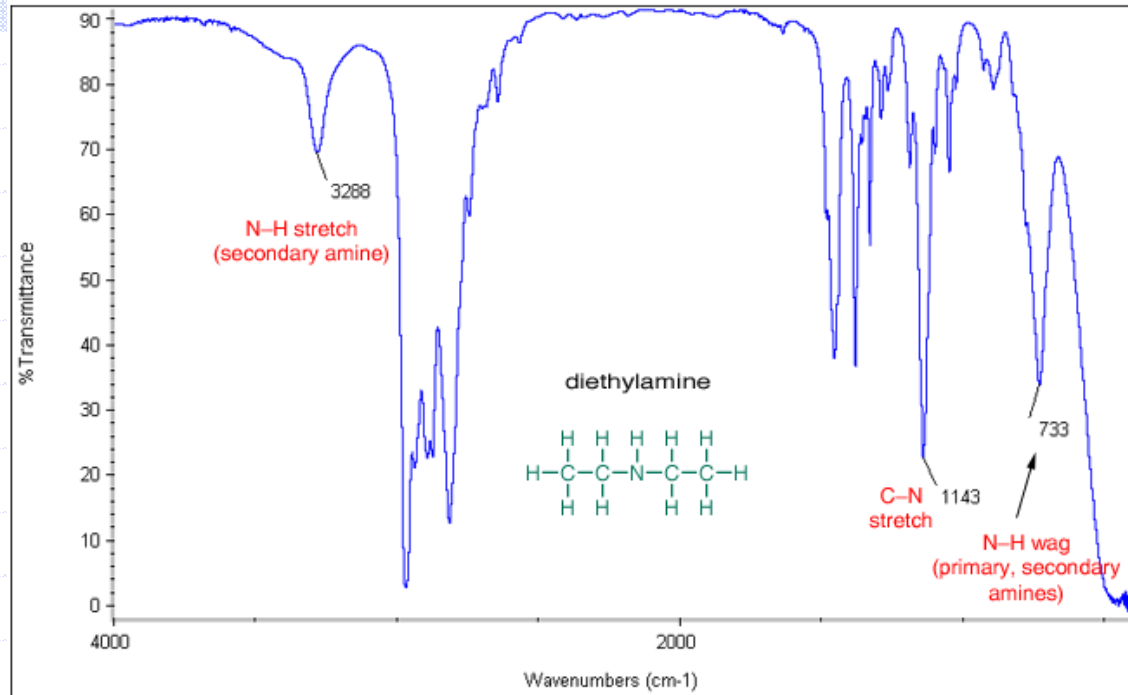
Ketone IR Data



Carboxylic Acid IR Data



Amine IR Data



Sources for IR Data

- Organic Chemistry at CU Boulder
 - Visit the site for tutorials and practice problems

